Command Index

Input

- Processed NMR data
 - o NMRPipe
 - o Felix
 - o Varian VNMR
 - Bruker XWinNMR and UXNMR
- <u>UCSF NMR format</u>
- Sparky spectrum annotation (aka "save") files
- Sparky project files

Output

- Peak lists
- Chemical shift list
- Chemical shift table

File commands

fo open UCSF NMR data, a Felix matrix, or a Sparky spectrum file

fs save a Sparky spectrum annotation file

<u>file save as...</u> fa save spectrum with a new name

<u>project open...</u> jo open several spectra at once

<u>project save</u> js save all spectra

project save as... ja save project with a new name

preferences... pf miscellaneous settings

quit qt

View commands

axes in Hertz xh display view scale axes in Hz

<u>axes in ppm</u> xp display view scale axes in parts per million

axes show index xd show data index values on view scales

<u>axis nucleus types</u> xa show nucleus type (1H, 13C, 15N) on axes <u>axis roll</u> xr exchange axes keeping center point of fixed

<u>axis transpose</u> xx zoom to cross-diagonal region of spectrum

center view on peak vc center a view on the selected peak

orthogonal views or show 3 orthogonal views of a 3-D spectrum

region goto rg zoom to a named region region tool... rt name regions of a spectrum

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renumber view rv renumber view name to use lowest available suffix number

show axis scales vs show scales (ppm, hz, or index units) along view axes

show grids gs toggle display of grids show labels ls toggle display of labels show lines is toggle display of lines

show ornaments os toggle display of all ornaments

show peaks ps toggle display of peaks

show peak groups xs toggle display of peak groups

show peak info vp show peak position / height / linewidth in status bar

show resonances vR show resonances along edge of spectrum

vb show scrollbars for view windows show scrollbars

show slices vS show 1-D data cross-sections along edge of spectrum

view duplicate vd make another view window

view hide vh undisplay a view

view redraw vr redraw the view (in case it gets messed up)

view settings... vt set crosshairs, aspect ratio, slices, ...

zoom full zf show entire spectrum zi zoom in by a factor of 2 zoom in zo zoom out by a factor of 2 zoom out

zd move down a plane in a 3D spectra zoom down zoom up zu move up a plane in a 3D spectra zp zoom to the previously shown region zoom previous

zn reverse of zoom previous (zp) command zoom next

Peak commands

copy

adjust peak w1,w2,w3,w4 frequency one sweepwidth add sweepwidth a1 a2 a3 a4

downfield

A1 A2 A3 adjust peak w1,w2,w3,w4 frequency one sweepwidth subtract sweepwidth

A4 upfield

u1 u2 u3 u4 reflect upfield reflect peak w1,w2,w3,w4 frequency about upfield boundary

reflect peak w1,w2,w3,w4 frequency about downfield d1 d2 d3 d4

reflect upfield boundary

assignment copy remember peak assignments for assignment paste ac

assignment delete delete the assignments of selected peaks aD

assignment paste aP paste assignments onto peaks in this spectrum

assignment paste & label copy assignments and show labels ap

crossdiagonal assignment aX copy assignments from crossdiagonal peaks

assignment tool... make assignments at

delete unused resonances delete resonances not used in any peak assignments dr

integration tool... it select integration method

sum over box method ib switch to box integration method

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sum over ellipse method	ie	switch to ellipse integration method
Gaussian fit method	ig	switch to Gaussian fit integration
Lorentzian fit method	il	switch to Lorentzian fit integration
integrate selected peaks	pi	
ornament copy	oc	record ornaments for future paste operation
ornament paste	op	paste ornaments into this spectrum
crossdiagonal ornament copy	_	copy ornaments across diagonal of 2D homonuclear spectrum
center peaks	pc	center selected peaks at local maxima or minima.
estimate linewidths	pe	get linewidth of selected peaks as width at half max
group peaks	pg	create a peak group from selected peaks
update heights	ph	reread peak heights from NMR data file
label peak	pl	put a label on a peak using a dialog
<u>label peaks</u>	lb	put assignment labels on selected peaks
unlabel peaks	lB	Remove labels from selected peaks
unoverlap labels	lu	move labels so they don't overlap each other
right offset labels	lr	move labels so they are to the right of peak markers
lock peaks	pk	prevent peaks from moving when integrated
select all peaks	pa	select all peaks in a spectrum
select fully assigned	pF	select fully assigned peaks
select partially assigned	pP	select partially assigned peaks
select unassigned	pN	select unassigned peaks
select by color	pC	select peaks by color
invert peak selection	pI	invert peak selection
select aliased	pA	select aliased peaks
select intra-residue	pR	select i to i assigned peaks
select sequential	pS	select i to i+1 assigned peaks
select medium range	pM	select i to i+2, i+3 or i+4 assigned peaks
select long range	pL	select i to i+5, i+6, assigned peaks
unintegrate peaks	pU	forget that a peak has been integrated
unlock peaks	pu	allow selected peaks to move when integrated
undo	eu	undo last peak move, deletion, or integration
w1 resonance peaks	r1	list assigned peaks with selected peak w1 resonance
w2 resonance peaks	r2	show assigments with selected peak w2 resonance
w3 resonance peaks	r3	show assigments with selected peak w3 resonance

Dialogs

<u>assignment...</u> at make assignments

assignment copy... co thresholds for copying assignments

assignment table... tb table of chemical shifts

<u>contour levels...</u> ct set contour levels and colors

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<u>integration...</u> it set integration method

midas... mi display assignments on a structure using Midas

<u>ornament...</u> ot change ornament colors and sizes

note... nt add notes to peaks

overlay views... ol overlay contours of one spectrum on another

<u>peak list...</u> It show a list of peaks for a spectrum

<u>peak picking...</u> kt set thresholds for find peak pointer mode pointer modes... pm show buttons to select pointer mode

predefined resonances... pd copy resonances from another spectrum

preferences... pf set global Sparky options

<u>print view...</u> pt print spectrum views to a Postscript printer

project view list... pv list of views, sizes, peak counts, ...

python... py Python shell for running your own programs region... rt name regions and apply operations to regions

rename resonances... rr rename atoms and groups

resonance list... rl list group/atom chemical shifts, standard deviations

spectrum... st set molecule and condition, and axis shifts

synchronize views... yt make views scroll in parallel

<u>view...</u> vt options controlling what is displayed in a view

Pointer Modes

select F1 click or drag to select or move peaks, labels, lines, ...

center F2 clicking centers view on point

add grid both F3 place vertical and horizontal grid lines

add grid horz F4 add a line extending across whole spectrum add grid vert F5 add a line extending across whole spectrum

add label F6 add a text label to a peak

add line F7 add a horizontal or vertical line between end points

find / add peak F8 click to place a peak or drag to find peaks

integrate F10 click or drag to integrate peaks

zoom F11 drag to select a new region to show

duplicate and zoom F12 drag to zoom and duplicate a view

assignment copy sh-F1 copy assignments from an already assigned spectrum

assignment guess sh-F2 make assignment if there is a unique guess

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